

THE MAXENT EXTENSION OF A QUANTUM GIBBS FAMILY, CONVEX GEOMETRY AND GEODESICS

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ABSTRACT. We discuss methods to analyze a quantum Gibbs family in the ultra-cold regime where the norm closure of the Gibbs family fails due to discontinuities of the maximum-entropy inference. The current discussion of maximum-entropy inference and irreducible correlation in the area of quantum phase transitions is a major motivation for this research. We extend a representation of the irreducible correlation from finite temperatures to absolute zero.

Keywords: – ground state, geodesic, convex geometry, maximum-entropy inference, quantum phase transition, irreducible correlation.

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1. INTRODUCTION

Closures of exponential families of probability distributions are a point of reference for our analysis of quantum Gibbs families. The classical setting of finite probability vectors belongs, in the form of diagonal matrices, to the non-commutative quantum setting of density matrices, which we synonymously call states. Weis and Knauf [24] found discontinuities of the maximum-entropy inference at the ‘boundary’ of a Gibbs family which consists of non-maximal rank states. The classical case is continuous because diagonal matrices commute.

An outstanding motivation for a ‘boundary’ analysis is the heuristic by Chen et. al [6] that a discontinuous maximum-entropy inference signals quantum phase transitions. Quantum phase transitions belong to ultra-cold physics, they appear for large inverse temperatures near the ‘boundary’ of a Gibbs family. Our asymptotic theory of Gibbs families supports the calculus of von Neumann’s maximum-entropy principle in quantum mechanics [19] which was proposed as an inference method by Jaynes [14].

A novelty concerns irreducible correlation, defined by Linden et al., and Zhou [16, 27] using the maximum-entropy principle, which can be interpreted as the amount of correlations caused by interactions between exactly k bodies, $k \in \mathbb{N}$. We write this function in terms of the divergence from a Gibbs family of local Hamiltonians. The maximal rank case for positive temperatures was done by Zhou [28], for algorithms see Niekamp et al. [17]. The classical theory was developed by Amari, and Ay et al. [1, 4].

We shed light on a proposal of Liu et al. [15] that irreducible correlation signals quantum phase transitions. For this we support an idea by Chen et al. [6] by pointing out that a discontinuous maximum-entropy inference and a discontinuous irreducible correlation are intimately connected. As an example we show that the irreducible correlation of three qubits is discontinuous. This follows also from the work of Linden et al. [16].

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2. CLOSURES OF STATISTICAL MODELS

We follow Csiszár and Matúš' ideas [11] about defining a maximum likelihood estimate (MLE) when the likelihood function has no maximum. This leads to closure concepts.

Let μ be a non-zero Borel measure on \mathbb{R}^n , $n \in \mathbb{N}$. The log-Laplace transform of μ is defined for $\vartheta \in \mathbb{R}^n$ by $\Lambda(\vartheta) := \ln \int_{\mathbb{R}^n} e^{\langle \vartheta, x \rangle} \mu(dx)$. The effective domain of Λ is $\text{dom}(\Lambda) := \{\vartheta \in \mathbb{R}^n \mid \Lambda(\vartheta) < \infty\}$ and the corresponding exponential family is

$$\mathcal{E} := \{Q_\vartheta \mid \frac{dQ_\vartheta}{d\mu} = e^{\langle \vartheta, \cdot \rangle - \Lambda(\vartheta)} \mu \text{ a.s., } \vartheta \in \text{dom}(\Lambda)\},$$

where $\frac{dQ_\vartheta}{d\mu}$ is the Radon-Nikodym derivative of Q_ϑ with respect to μ . The MLE of the mean a of an iid sample from a probability measure Q_ϑ with unknown parameter $\vartheta \in \text{dom}(\Lambda)$ is defined as a maximizer ϑ^* of the function

$$(1) \quad \vartheta \mapsto \langle \vartheta, a \rangle - \Lambda(\vartheta), \quad \vartheta \in \text{dom}(\Lambda).$$

If a is the mean of a distribution Q_θ then the choice $\vartheta^* = \theta$ maximizes (1) because of

$$[\langle \vartheta^*, a \rangle - \Lambda(\vartheta^*)] - [\langle \vartheta, a \rangle - \Lambda(\vartheta)] = D(Q_{\vartheta^*} \| Q_\vartheta), \quad \vartheta \in \text{dom}(\Lambda).$$

Here D is the Kullback-Leibler divergence which is an asymmetric distance, $D(P \| Q) := \int \ln \frac{dP}{dQ} dP$ if P is absolutely continuous with respect to Q and otherwise $D(P \| Q) := \infty$.

It is known [11] that for any $a \in \mathbb{R}^n$ where the supremum in (1), denoted by $\Psi^*(a)$, is finite, there exists a unique probability measure $R^*(a)$ such that

$$(2) \quad \Psi^*(a) - [\langle \vartheta, a \rangle - \Lambda(\vartheta)] \geq D(R^*(a) \| Q_\vartheta), \quad \vartheta \in \text{dom}(\Lambda).$$

The generalized MLE $R^*(a)$ is a natural generalization of the MLE ϑ^* and $R^*(a) = Q_{\vartheta^*}$ holds if ϑ^* exists [11]. Equation (2) shows that $R^*(a)$ lies in $\text{cl}^{\text{rI}}(\mathcal{E}) := \{P \mid \inf_{\vartheta \in \text{dom}(\Lambda)} D(P \| Q_\vartheta) = 0\}$, called rI-closure of \mathcal{E} ('rI' reads 'reverse I' [8]). The total variation $\delta(P, Q)$ between two Borel probability measures P, Q is bounded above by the divergence in the Pinsker inequality so the total variation closure contains $\text{cl}^{\text{rI}}(\mathcal{E})$.

An example of $\text{cl}^{\text{rI}}(\mathcal{E}) \subsetneq \text{cl}^{\text{rI}}(\text{cl}^{\text{rI}}(\mathcal{E}))$ for $n = 3$ is known [9]. The analogue of the closure operator cl^{rI} for a finite-level quantum system belongs to a topology, called rI-topology, and is idempotent [22] but the rI-topology is strictly finer than the norm topology. In the classical case (of finite support) the rI-topology equals the norm topology.

3. GROUND STATE LEVEL-CROSSINGS

We discuss limits of Gibbs families, ground state level-crossings of Hamiltonians and the heuristics by Chen et al. [6] regarding quantum phase transitions.

We consider the matrix algebra M_d , $d \in \mathbb{N}$, of complex $d \times d$ matrices with identity $\mathbb{1}$ and, for non-zero projections $p = p^2 = p^* \in M_d$, algebras $\mathcal{A} = pM_dp = \{pap \mid a \in M_d\}$. The real space of Hamiltonians $\mathcal{A}^{\text{h}} = \{a \in \mathcal{A} \mid a^* = a\}$ is a Euclidean space with the scalar product $\langle a, b \rangle = \text{tr}(ab)$. The Gibbs state of $H \in M_d^{\text{h}}$ at the inverse temperature $\beta > 0$ is given by $g_H(\beta) := e^{-\beta H} / \text{tr}(e^{-\beta H})$. The zero-temperature limit

$$(3) \quad g^\infty(H) := \lim_{\beta \rightarrow +\infty} g_H(\beta) = p / \text{tr}(p)$$

is a ground state of H . More precisely, p is the projection onto the ground state space of H , that is the eigenspace of H for the smallest eigenvalue.

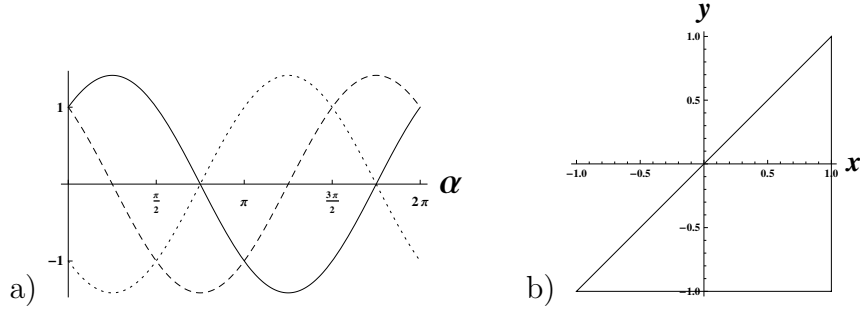


FIGURE 1. a) Eigenvalues of \tilde{H} with Type I level-crossing b) Triangle convex support \mathbb{L} .

Now we consider a sequence of Hamiltonians $H_i \in M_d^h$, $i = 1, \dots, r$, $r \in \mathbb{N}$. Similarly to the ground state $g^\infty(H)$ of H being a limit of the curve g_H , the ground states of the Hermitian pencil $H(\lambda) := \lambda_1 H_1 + \dots + \lambda_r H_r$, $\lambda = (\lambda_1, \dots, \lambda_r) \in \mathbb{R}^r$, are limits of the Gibbs family $\mathcal{E} := \{e^{H(\lambda)} / \text{tr}(e^{H(\lambda)}) \mid \lambda \in \mathbb{R}^r\}$. Both \mathcal{E} and the limits shall be studied in terms of expected values. Consider the state space $\mathcal{M}(\mathcal{A}) := \{\rho \in \mathcal{A} \mid \rho \succeq 0, \text{tr}(\rho) = 1\}$. The state space $\mathcal{M}_d := \mathcal{M}(M_d)$ of the full algebra represents the physical states of the quantum system ($\rho \succeq 0$ means that ρ is positive semi-definite). The expected value functional is $\mathbb{E} : M_d^h \rightarrow \mathbb{R}^r$, $a \mapsto (\langle H_1, a \rangle, \dots, \langle H_r, a \rangle)$. The convex support $\mathbb{L} := \mathbb{E}(\mathcal{M}_d)$ consists of all expected values [5, 8, 21].

The von Neumann entropy $H(\rho) := -\text{tr} \rho \log(\rho)$ is a measure of the uncertainty in $\rho \in \mathcal{M}_d$ [14, 20]. The maximum-entropy inference is the map

$$\rho^* : \mathbb{L} \rightarrow \mathcal{M}_d, \quad \alpha \mapsto \text{argmax}\{H(\rho) \mid \rho \in \mathcal{M}_d, \mathbb{E}(\rho) = \alpha\}.$$

According to Jaynes [14] the state $\rho^*(\alpha)$ has expectation value α and minimal other information. The Gibbs family \mathcal{E} contains all states $\rho^*(\alpha)$ of maximal rank d . Wichmann [26] has shown that ρ^* restricted to the relative interior $\text{ri}(\mathbb{L})$ of \mathbb{L} (interior in the affine hull) is a real analytic parametrization of \mathcal{E} , so $\rho^*(\text{ri}(\mathbb{L})) = \mathcal{E}$ holds.

We discuss ground state limits of \mathcal{E} and their expected values on the relative boundary $\mathbb{L} \setminus \text{ri}(\mathbb{L})$ of \mathbb{L} . For $r = 2$ Hamiltonians we draw \mathbb{L} in x - y -coordinates and we parametrize $\tilde{H}(\alpha) := H(\cos(\alpha), \sin(\alpha))$, $\alpha \in \mathbb{R}$. We use the Pauli matrices

$$\sigma_1 := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

We denote the standard basis of \mathbb{C}^3 by e_1, e_2, e_3 and we write v^*w for the inner product of $v, w \in \mathbb{C}^3$ and vw^* for the linear map $vw^*(z) := (w^*z) \cdot v$ defined for $z \in \mathbb{C}^3$.

The first example of a level-crossing has a discontinuous ground state with discontinuous expected value and is called Type I level-crossing by Chen et al. [6]. It occurs in the commutative case of finite systems and corresponds to a first-order phase transition.

Example (Type I level-crossing). Let $H_1 = \sigma_3 \oplus 1$ and $H_2 = \sigma_3 \oplus (-1)$, the direct sums being embedded as block diagonal matrices into M_3 . The ground state $g^\infty(\tilde{H}(\alpha)) = p / \text{tr}(p)$ stays at $p = e_2 e_2^*$ for $-\frac{1}{4}\pi < \alpha < \frac{1}{2}\pi$ and jumps to $(e_2 e_2^* + e_3 e_3^*) / 2$ at $\alpha = \frac{1}{2}\pi$. Thereby the expected value $\mathbb{E}(g^\infty(\tilde{H}(\alpha)))$ jumps from $(-1, -1)$ to $(0, -1)$. See Figure 1.

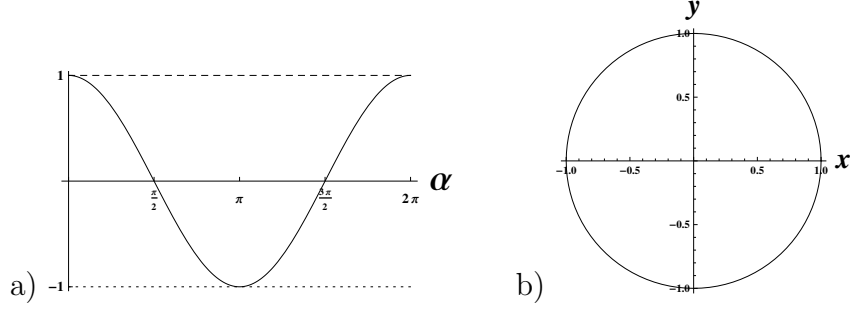


FIGURE 2. a) Eigenvalues of \tilde{H} with Type II level-crossing b) Disk convex support \mathbb{L} .

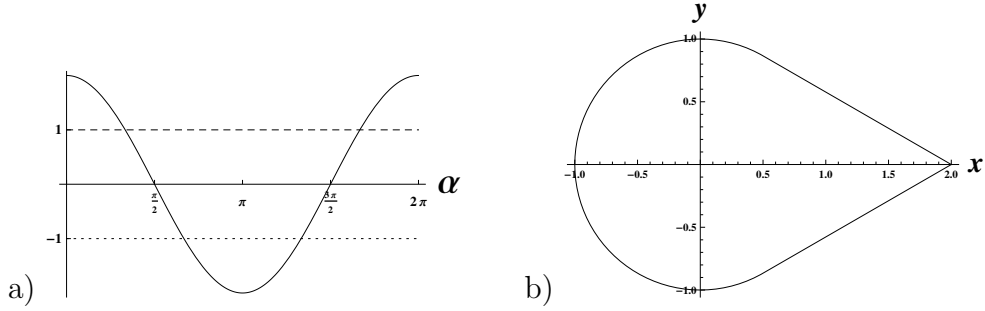


FIGURE 3. a) Eigenvalues of \tilde{H} with Type I level-crossing b) Drop shape convex support \mathbb{L} (convex hull of the unit disk and the point $(2,0)$) with two non-exposed points where the boundary segments meet the disk.

The second example of a level-crossing has a discontinuous ground state with continuous expected value and is called Type II level-crossing [6]. We will see it implies a discontinuous ρ^* . In the thermodynamic limit a Type II level-crossing is associated with a continuous phase transition which includes many quantum phase transitions.

Example (Type II level-crossing). Let $H_1 = \sigma_1 \oplus 1$ and $H_2 = \sigma_2 \oplus 0$. The ground state is $g^\infty(\tilde{H}(\alpha)) = v(\alpha)v(\alpha)^*$ for $\alpha \neq \pi \bmod 2\pi$ where $v(\alpha) = (1, -e^{i\alpha}, 0)/\sqrt{2}$ and $g^\infty(\tilde{H}(\pi)) = (v(\pi)v(\pi)^* + e_3e_3^*)/2$. The expected value is $\mathbb{E}(g^\infty(\tilde{H}(\alpha))) = -(\cos(\alpha), \sin(\alpha))$ for all α . See Figure 2.

The last example, a Type I level-crossing, demonstrates a convex geometric feature.

Example (Drop shape convex support). Let $H_1 = \sigma_1 \oplus 2$ and $H_2 = \sigma_2 \oplus 0$. Ground states are discussed in Sec. 33(3) in [21]. See Figure 3.

4. THE MAXENT EXTENSION

We construct an extension of a Gibbs family \mathcal{E} for which a Pythagorean theorem holds. As a corollary the extension is the set of maximum-entropy states.

Maximum-entropy states are unique so there is only one extension with Pythagorean theorem. We begin with a geodesic closure defined by adding states with maximal

support on the ground state space of some $H(\lambda)$. Non-exposed points of \mathbb{L} force us to include states without maximal support on the ground state space of any $H(\lambda)$.

The six limit points of the form (3) in the first example above define six expected values. They do not cover the relative boundary of the triangle \mathbb{L} so Wichmann's equation $\mathbb{E}(\mathcal{E}) = \text{ri}(\mathbb{L})$ shows that a larger class of curves is needed. A (+1)-geodesic [2] in the manifold of invertible states in \mathcal{M}_d is defined for $H_0, H \in M_d^h$ by

$$g_{H_0, H}(t) := e^{H_0 + tH} / \text{tr}(e^{H_0 + tH}), \quad t \in \mathbb{R}.$$

If p is the projection onto the ground state space of $-H$ then Lemma 6.13 in [22] shows

$$(4) \quad \lim_{t \rightarrow \infty} g_{H_0, H}(t) = pe^{pH_0p} / \text{tr}(pe^{pH_0p}).$$

The (+1)-geodesic closure $\text{cl}^{(+1)}(\mathcal{E})$ of the Gibbs family \mathcal{E} is defined as the union of (+1)-geodesics in \mathcal{E} with their limit points. Let $p \in M_d$ be a non-zero projection and put $\mathcal{E}_p := \{pe^{pH(\lambda)p} / \text{tr}(pe^{pH(\lambda)p}) \mid \lambda \in \mathbb{R}^r\}$. The limit (4) shows $\text{cl}^{(+1)}(\mathcal{E}) = \bigcup_p \mathcal{E}_p$ where the union is over projections p onto a ground state space of some $H(\lambda)$, $\lambda \in \mathbb{R}^r$.

Convex geometry prevents the inclusion $\mathbb{E}(\text{cl}^{(+1)}(\mathcal{E})) \subset \mathbb{L}$ from always being an equality, a detailed discussion is Sec. 6.6 in [22]. If $C \neq \emptyset$ is a compact convex subset of a Euclidean space X then $u \in X$ defines an exposed face $F_C(u) := \text{argmax}\{\langle c, u \rangle \mid c \in C\}$ of C . Exposed faces of \mathcal{M}_d have the form

$$(5) \quad F_{\mathcal{M}_d}(H) = \mathcal{M}(pM_dp), \quad H \in M_d^h,$$

where p is the projection onto the ground state space of $-H$ [21]. Exposed faces of the convex support satisfy

$$(6) \quad \mathbb{E}|_{\mathcal{M}_d}^{-1}(F_{\mathbb{L}}(\lambda)) = F_{\mathcal{M}_d}(H(\lambda)), \quad \lambda \in \mathbb{R}^r.$$

For example in Fig. 1b) we have for $\alpha \in (\frac{3}{4}\pi, \frac{3}{2}\pi)$ and $\lambda = (\cos(\alpha), \sin(\alpha))$ exposed faces $F_{\mathbb{L}}(\lambda) = \{(-1, -1)\}$ and $F_{\mathcal{M}_3}(H(\lambda)) = \{e_2 e_2^*\}$.

Wichmann's equality $\rho^*(\text{ri}(\mathbb{L})) = \mathcal{E}$ with \mathbb{L} replaced by an exposed face F of \mathbb{L} and with \mathcal{E} replaced by \mathcal{E}_p , where $p = p(F)$ is defined in (5), (6), implies that $\mathbb{E}(\text{cl}^{(+1)}(\mathcal{E}))$ covers only points of \mathbb{L} which belong to the relative interior of an exposed face of \mathbb{L} . Points not having this form, see Fig. 3b), are called non-exposed points.

Non-exposed points—and higher-dimensional analogues—have to be treated separately, see Sec. 6.2 in [22] for details. A face of a compact convex subset C of a Euclidean space is a convex subset F of C such that every segment in C which meets with its relative interior the set F belongs to F . Let \mathcal{P} denote the set of projections p defined implicitly by $\mathcal{M}(pM_dp) = \mathbb{E}|_{\mathcal{M}_d}^{-1}(F)$ for non-empty faces F of \mathbb{L} . Then the extension

$$\text{ext}(\mathcal{E}) := \bigcup_{p \in \mathcal{P}} \mathcal{E}_p$$

induces a bijection $\mathbb{E}|_{\text{ext}(\mathcal{E})} : \text{ext}(\mathcal{E}) \rightarrow \mathbb{L}$ and we have $\mathcal{E} \subset \text{cl}^{(+1)}(\mathcal{E}) \subset \text{ext}(\mathcal{E})$. For $\rho \in \mathcal{M}_d$ we denote by $\pi_{\mathcal{E}}(\rho)$ the unique state in $\text{ext}(\mathcal{E})$ such that $\mathbb{E}(\rho) = \mathbb{E}(\pi_{\mathcal{E}}(\rho))$. So $\pi_{\mathcal{E}}$ is a projection from \mathcal{M}_d onto $\text{ext}(\mathcal{E})$.

Pythagorean and projection theorems will show that $\text{ext}(\mathcal{E})$ is a useful extension. The relative entropy of $\rho, \sigma \in \mathcal{M}_d$, also known as divergence, is defined by $D(\rho, \sigma) := \text{tr} \rho(\log(\rho) - \log(\sigma))$ if $\ker(\sigma) \subset \ker(\rho)$. Otherwise $D(\rho, \sigma) = +\infty$. The divergence, an asymmetric distance, is non-negative and zero only for identical arguments [20].

Theorem (Pythagorean theorem, Thm. 6.12 in [22]). *Let $\rho \in \mathcal{M}_d$ and $\sigma \in \text{ext}(\mathcal{E})$. Then $D(\rho, \sigma) = D(\rho, \pi_{\mathcal{E}}(\rho)) + D(\pi_{\mathcal{E}}(\rho), \sigma)$ holds.*

This theorem extends results by Petz, and Amari and Nagaoka [18, 2] to non-maximal rank states and classical results by Csiszár and Matúš [8] to quantum states.

The Pythagorean theorem with $\sigma = \mathbb{1}/d$ shows $\pi_{\mathcal{E}}(\rho^*(\alpha)) = \rho^*(\alpha)$ for $\alpha \in \mathbb{L}$, that is $\rho^*(\mathbb{L}) = \text{ext}(\mathcal{E})$ holds (details in Sec. 3.4 in [22]). In the Type II level-crossing example the ground states $g^\infty(\tilde{H}(\alpha))$ belong to $\text{cl}^{(+1)}(\mathcal{E}) \subset \rho^*(\mathbb{L})$. As $g^\infty(\tilde{H}(\alpha))$ is discontinuous at $\alpha = \pi$ and has continuous expected values, ρ^* is discontinuous at $\mathbb{E}(g^\infty(\tilde{H}(\pi))) = (1, 0)$. This proof is similar to Exa. 1 in [6], see [24, 23] for other proofs.

5. THE REVERSE I-CLOSURE

A projection theorem allows us to represent the divergence from a Gibbs family as a difference of von Neumann entropies. This applies to the irreducible correlation.

The divergence from a subset $X \subset \mathcal{M}_d$ is $d_X : \mathcal{M}_d \rightarrow [0, \infty]$, $\rho \mapsto \inf\{D(\rho, \sigma) \mid \sigma \in X\}$. Since $\mathbb{1}/d \in \mathcal{E}$ holds, the divergence $d_{\mathcal{E}}$ has on \mathcal{M}_d the global upper bound $\log(d)$.

Theorem (Projection theorem, Thm. 6.16 in [22]). *Let $\rho \in \mathcal{M}_d$. Then $D(\rho, \cdot)$ has on $\text{ext}(\mathcal{E})$ a unique local and global minimum at $\pi_{\mathcal{E}}(\rho)$ and $d_{\mathcal{E}}(\rho) = D(\rho, \pi_{\mathcal{E}}(\rho))$ holds.*

This theorem shows that $\text{ext}(\mathcal{E})$ is the rI-closure $\{\rho \in \mathcal{M}_d \mid d_{\mathcal{E}}(\rho) = 0\}$ of \mathcal{E} . The proof of the theorem needs Grünbaum's [13] notion of poonem of \mathbb{L} (Sec. 3.6 in [22]) which is equivalent to face of \mathbb{L} and to access sequence [10]. Recursively defined, \mathbb{L} is a poonem of \mathbb{L} and all exposed faces of poonems of \mathbb{L} are poonems of \mathbb{L} . In Figure 3b) the non-exposed points are poonems because they are exposed faces of a segment.

Consider the Gibbs family $\mathcal{E}(\mathcal{H}) := \{e^H/\text{tr}(e^H) \mid H \in \mathcal{H}\}$ of a subspace $\mathcal{H} \subset M_d^{\text{h}}$. If a basis of \mathcal{H} is chosen then expectation \mathbb{E} , convex support \mathbb{L} , maximum-entropy inference ρ^* and projection $\pi_{\mathcal{E}(\mathcal{H})}$ are defined (\mathbb{E} , \mathbb{L} and ρ^* do not depend much on the basis and $\pi_{\mathcal{E}(\mathcal{H})}$ is invariant under basis change). The projection theorem and the Pythagorean theorem (with $\sigma = \mathbb{1}/d$) show for $\rho \in \mathcal{M}_d$ the equality

$$(7) \quad \begin{aligned} d_{\mathcal{E}(\mathcal{H})}(\rho) &= D(\rho, \pi_{\mathcal{E}(\mathcal{H})}(\rho)) = D(\rho, \mathbb{1}/d) - D(\pi_{\mathcal{E}(\mathcal{H})}(\rho), \mathbb{1}/d) \\ &= H(\pi_{\mathcal{E}(\mathcal{H})}(\rho)) - H(\rho). \end{aligned}$$

Now we consider a flag $\mathcal{H}_1 \subset \dots \subset \mathcal{H}_N \subset M_d^{\text{h}}$, $N \in \mathbb{N}$, and $C_k(\rho) := H(\pi_{\mathcal{E}(\mathcal{H}_{k-1})}(\rho)) - H(\pi_{\mathcal{E}(\mathcal{H}_k)}(\rho))$, $k = 2, \dots, N$. We obtain $C_k = d_{\mathcal{E}(\mathcal{H}_{k-1})} - d_{\mathcal{E}(\mathcal{H}_k)}$ from (7). Often $\mathcal{H}_N = \mathcal{A}^{\text{h}}$ holds. Then $d_{\mathcal{E}(\mathcal{H}_N)} \equiv 0$ follows and we have $d_{\mathcal{E}(\mathcal{H}_1)} = C_2 + \dots + C_N$.

We turn to the irreducible k -body correlation, $k = 2, \dots, N$, of a quantum system composed of $N \in \mathbb{N}$ units. Let the unit $i \in [N] := \{1, \dots, N\}$ have algebra \mathcal{A}_i and the total system have the tensor product algebra $\mathcal{A} := \bigotimes_{i \in [N]} \mathcal{A}_i$. For $A \subset [N]$ let $\mathcal{A}_A := \bigotimes_{i \in A} \mathcal{A}_i$ and let $\mathbb{1}_A$ be the identity in \mathcal{A}_A . A k -local Hamiltonian H is a sum of terms of the form $\mathbb{1}_{[N] \setminus A} \otimes b$ for $b \in \mathcal{A}_A^{\text{h}}$ where $A \subset [N]$ has cardinality $|A| \leq k$.

Let \mathcal{H}_k be the space of k -local Hamiltonians. Then C_k is the k -body irreducible correlation [16, 27]. If $A \subset [N]$ and $\rho \in \mathcal{M}(\mathcal{A})$ then $\langle X, \rho_A \rangle = \langle X \otimes \mathbb{1}_{[N] \setminus A}, \rho \rangle$, $X \in \mathcal{A}_A^{\text{h}}$, defines a marginal ρ_A . The expectation $\langle \rho, H \rangle$ of a k -local Hamiltonian H can be

computed from the k -reduced density matrices $\rho^{(k)} = (\rho_A)_{A \subset [N], |A|=k}$ (k -RDM's). So $\pi_{\mathcal{E}(\mathcal{H}_k)}(\rho) = \rho^*(\rho^{(k)})$ is well-defined and, according to Jaynes [14], $\rho^*(\rho^{(k)})$ represents the k -RDM's of ρ in the most unbiased way because it has minimal other information. Zhou [27] has interpreted $C_k(\rho)$ as the amount of k -body correlations in ρ which are no $(k-1)$ -body correlations by arguing that correlation decreases uncertainty. The total correlation $I(\rho) := \sum_{i \in [N]} H(\rho_{\{i\}}) - H(\rho)$ is also known as multi-information [3].

Since $I = d_{\mathcal{E}(\mathcal{H}_1)}$ holds [25] we have, as in the paragraph of (7), for $k = 2, \dots, N-1$

$$(8) \quad C_k = d_{\mathcal{E}(\mathcal{H}_{k-1})} - d_{\mathcal{E}(\mathcal{H}_k)}, \quad C_N = d_{\mathcal{E}(\mathcal{H}_{N-1})} \quad \text{and} \quad I = C_2 + \dots + C_N.$$

The projection theorem shows, continuing Jaynes' view, that $d_{\mathcal{E}(\mathcal{H}_{k-1})}(\rho)$ is the divergence from the set of most unbiased representatives of $(k-1)$ -RDM's. So it is reasonable to interpret it as the amount of correlations in ρ caused by interactions of k or more bodies. Then C_k is the amount of correlations in ρ caused by interactions of exactly k bodies. No information-theoretic proof exists for this interpretation except for the total correlation [12].

We point out that $C_3 = d_{\mathcal{E}(\mathcal{H}_2)}$ is discontinuous for three qubits. Exa. 6 in [6] shows that $\rho^*(\rho^{(2)})$ is discontinuous at some $\rho^{(2)} = (\rho_{\{2,3\}}, \rho_{\{1,3\}}, \rho_{\{1,2\}})$ so Lemma 5.14(2) in [23] shows that $d_{\mathcal{E}(\mathcal{H}_2)}$ is discontinuous at some $\sigma \in \mathcal{M}(\mathcal{A})$ with $\sigma^{(2)} = \rho^{(2)}$. While Lemma 5.14(2) in [23] applies to any composite system and to $\rho^*(\rho^{(k)})$ for any k , the three qubit discontinuity follows also from the fact [16] that $C_3(\rho) = 0$ holds for pure states ρ which are not local unitary equivalent to $a|000\rangle + b|111\rangle$. Classically, $d_{\mathcal{E}}$ is continuous for any Gibbs family \mathcal{E} , see Sec. 6.6 in [22], so C_k is continuous for all k .

6. (-1) -GEODESICS

We now consider geodesics in the Gibbs family \mathcal{E} which, unlike the $(+1)$ -geodesics, generate the set of maximum-entropy states $\rho^*(\mathbb{L})$ with their limits.

A topological analysis [23], related to multi-valued maps [7], shows the following.

Remark (Polytopes, Thm. 4.9 and Coro. 4.13 in [23]). If $X \subset \mathbb{L}$ is a polytope then $\rho^*|_X$ is continuous. So, if $s \subset \text{ri}(\mathbb{L})$ is a segment with norm closure \bar{s} then $\rho^*|_{\bar{s}}$ is continuous.

An unparametrized (-1) -geodesic in \mathcal{E} is defined as the image $\rho^*(s)$ of a relative open segment $s \subset \text{ri}(\mathbb{L})$, see [2]. This definition is consistent by Wichmann's equation $\rho^*(\text{ri}(\mathbb{L})) = \mathcal{E}$. Since $\rho^*|_{\bar{s}}$ is continuous we get the following.

Theorem (Geodesic closure, Thm. 5.10 in [23]). *The union of (-1) -geodesics in \mathcal{E} and their limit points equals $\rho^*(\mathbb{L})$.*

7. CONCLUSION

We have discussed methods towards an asymptotic theory of quantum Gibbs families in the ultra-cold regime. Some properties, such as the continuity of ρ^* , break down from finite temperatures to absolute zero while others, such as the Pythagorean and projection theorem, extend. In this article we have extended a representation of the irreducible correlation.

Comparisons to models of quantum statistical physics will show how to make further developments. On the other hand basic mathematical questions are widely

unexplored such as the continuity of the irreducible correlation of three qubits or the continuity of the maximum-entropy inference beyond the case of two qutrit Hamiltonians.

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